Hexachloro-1,3-butadiene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1720 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.68e-01

Confidence level: 6.93e-01

Nearest Neighbors from the Training Set

Image not found
Hexachlorobenzene
Measured: 5500
Predicted: 6740

Image not found
Pentachlorobenzene
Measured: 3160
Predicted: 5490

Image not found
Pentachlorophenol
Measured: 20000
Predicted: 15100

Image not found
Tetrachloroethylene
Measured: 251
Predicted: 170

Image not found
1,2-Dibromo-3-chloropropane
Measured: 70.8
Predicted: 84.1